

Solving the Coulomb scattering problem using the complex scaling method

M. V. VOLKOV^{1,2} ^(a) N. ELANDER¹ E. YAREVSKY² and S. L. YAKOVLEV²

¹ Department of Physics, AlbaNova University Center, Stockholm University, 106 91 Stockholm, Sweden

² Department of Computational Physics, St Petersburg State University, 198504 St Petersburg, Russia

PACS 03.65.Nk – Scattering theory

PACS 34.80.Bm – Elastic scattering

Abstract. - Based on the work of Nuttall and Cohen [Phys. Rev. **188** (1969) 1542] and Resigno *et al.* [Phys. Rev. A **55** (1997) 4253] we present a rigorous formalism for solving the scattering problem for long-range interactions without using exact asymptotic boundary conditions. The long-range interaction may contain both Coulomb and short-range potentials. The exterior complex scaling method, applied to a specially constructed inhomogeneous Schrödinger equation, transforms the scattering problem into a boundary problem with zero boundary conditions. The local and integral representations for the scattering amplitudes have been derived. The formalism is illustrated with numerical examples.

Introduction. – Few-body systems held together by a mutual Coulomb interaction are of great interest in many areas of quantum physics. However, solving the Coulomb scattering problem is a very difficult task both from the theoretical as well as the computational points of view due to the long-range character of the Coulomb interaction. The asymptotic boundary conditions for the wave function at large separations between particles are already complicated for the few-body scattering problem with short-range interactions [1]. They become even more complicated for the long-range case when the Coulomb potential is present in the interaction [2]. Therefore, a method which allows the problem to be solved without explicit use of the asymptotic form of the wave function is of great interest from both the theoretical and computational points of view.

One of such methods was proposed by Nuttal and Cohen [3]. The approach is based on the complex scaling theory [4]. The idea can briefly be formulated as follows.

The Schrödinger equation is recast into its inhomogeneous (driven) form by splitting the wave function into the sum $\Psi = \Psi_{in} + \Psi_{sc}$ of the incident Ψ_{in} and scattered Ψ_{sc} waves as

$$(H_0 + V - E)\Psi_{sc} = -V\Psi_{in}. \quad (1)$$

The scattered wave is the subject of the purely outgoing

boundary condition $\Psi_{sc} \propto \exp\{i\sqrt{E}r\}$. Then, after the complex scaling transformation, the original real coordinate will be replaced by z , $\Im z > 0$, implying that the scattered wave vanishes exponentially $\Psi_{sc} \propto \exp\{i\sqrt{E}z\}$ as $|z| \rightarrow \infty$. This property is consistent with Eq. (1) as long as the right hand side term $V(z)\Psi_{in}(z)$ vanishes as $|z| \rightarrow \infty$. This condition is always fulfilled if the potential has only finite range. Otherwise only exponentially decreasing potentials $V(r) \propto \exp\{-\mu r\}$ are admissible [3]. The problem is that the incident wave Ψ_{in} always contains the incoming wave $\exp\{-i\sqrt{E}r\}$ in addition to the outgoing wave. This wave increases in magnitude after the complex scaling as $|z| \rightarrow \infty$. This increase can only be compensated for if the potential decreases exponentially with increasing z .

In the two body scattering problem the Coulomb potential can be implemented into the approach just discussed if it is included in the Hamiltonian H_0 , while V assumes the short-range part of the interaction. In this case the incident wave Ψ_{in} is represented by the Coulomb wave function, which is known analytically. This approach has been successfully used for calculations in atomic [5] and nuclear [6] physics. Unlike the two body case, the analytic solution for the Coulomb problem does not exist if three or more particles are involved in the scattering process. Therefore, this version of the method does not work for more than two charged particles.

The mathematics is only valid for potentials V , which

^(a)E-mail: miha@physto.se

at large distances do not decrease slower than exponentially. Nevertheless, it was found by McCurdy, Rescigno and coworkers [5, 7, 8] that the method can give good results for the slow decreasing potentials when applied in the following way. Let R be a parametrical radius chosen such that $V(r) \ll E$ for $r \geq R$. Then Eq. (1) can be approximated by

$$(H_0 + V - E)\Psi_{sc} = -V_R\Psi_{in}. \quad (2)$$

Here the finite-range potential V_R is introduced in such a way that $V_R = V$, if $r \leq R$, and $V_R = 0$ otherwise. The exterior complex scaling (ECS) [9, 10] is then applied to Eq. (2) instead of Eq. (1). The mathematical properties of this interpretation of the method have not been studied earlier to the best of our knowledge. Furthermore, its extension to the Coulomb case remained questionable. However, the definite success in applying this method to important and complicated problems (see papers [5, 8], [11] and references therein) makes a detailed study urgent.

The aim of the present note is to set the above formulated approximative approach on a mathematically solid basis. A new formalism for solving the scattering problem with long-range interactions, including the Coulomb potential, is presented. The new formalism is based on an inhomogeneous Schrödinger equation with the right hand side containing the finite range potential V_R as in Eq. (2). The present contribution will open the way to further rigorous extensions of the scattering problem with more than two particles.

In this study we consider the scattering problem for a two body system with a central potential in the center of mass frame. Therefore, the Schrödinger equation for one partial wave $\Psi_\ell(k, r)$, with angular momentum ℓ and momentum $k = \sqrt{E}$, is considered.

Scattering problem and driven Schrödinger equation. – Let Ψ_ℓ be the wave function for a given orbital momentum ℓ . It is the solution to the partial wave Schrödinger equation $(H_\ell + V - k^2)\Psi_\ell = 0$ with the “free” Hamiltonian $H_\ell = -\partial_r^2 + \ell(\ell+1)/r^2$ and the interaction potential $V(r) = 2k\eta/r + V_s(r)$. V_s is assumed to vanish faster than $1/r^2$ at large distances, and is referred to as the short-range potential in this note.

The scattering solution is defined by the boundary condition $\Psi_\ell(k, 0) = 0$ and the asymptotics as $r \rightarrow \infty$ yielding

$$\Psi_\ell(k, r) \sim e^{i\sigma_\ell} F_\ell(\eta, kr) + \mathcal{A} u_\ell^+(\eta, kr). \quad (3)$$

Here $u_\ell^\pm = e^{\mp i\sigma_\ell}(G_\ell \pm iF_\ell)$, where $F_\ell(G_\ell)$ is the regular (irregular) Coulomb wave function [12], and $\sigma_\ell = \arg \Gamma(1 + \ell + i\eta)$ is the Coulomb phase shift. The scattering amplitude

$$\mathcal{A} = e^{2i\sigma_\ell} \frac{e^{2i\delta_\ell} - 1}{2i} \quad (4)$$

is determined by the phase shift δ_ℓ , which is due to the presence of the potential V_s .

In order to reformulate the problem in terms of a driven Schrödinger equation, the potential V is split into the sum $V = V_R + V^R$ containing the just introduced interior V_R part and the exterior V^R part. The splitting of the wave function $\Psi_\ell = \Psi_R + \Psi^R$ leads to the driven equation

$$(H_\ell + V - k^2)\Psi_R = -V_R\Psi^R \quad (5)$$

provided that Ψ^R obeys the Schrödinger equation with the exterior potential

$$(H_\ell + V^R - k^2)\Psi^R = 0. \quad (6)$$

The solution to Eq. (6) is constructed in such a way that it incorporates the incident wave $e^{i\sigma_\ell} F_\ell$. Therefore, Ψ^R has to represent the regular solution at $r = 0$ such that $\Psi^R(k, 0) = 0$ and has to fulfill the asymptotics that is similar to (3)

$$\Psi^R(k, r) \sim e^{i\sigma_\ell} F_\ell(\eta, kr) + \mathcal{A}^R u_\ell^+(\eta, kr) \quad (7)$$

with the amplitude \mathcal{A}^R given by

$$\mathcal{A}^R = e^{2i\sigma_\ell} \frac{e^{2i\delta^R} - 1}{2i}. \quad (8)$$

Note that the asymptotics (7) is relevant to that part of the function $\Psi^R(k, r)$, which is defined for $r > R$. For $r \leq R$ the potential V^R vanishes ($V^R(r) = 0$). Therefore, the function $\Psi^R(k, r)$ must be proportional to the Riccati-Bessel function j_ℓ [12]:

$$\Psi^R(k, r) = a^R j_\ell(kr). \quad (9)$$

In order to determine the function $\Psi^R(k, r)$ for $r > R$ it is useful to rewrite the asymptotics (7) in terms of Coulomb functions u_ℓ^\pm

$$\Psi^R(k, r) \sim \frac{1}{2i} [-u_\ell^-(\eta, kr) + S^R u_\ell^+(\eta, kr)], \quad (10)$$

where $S^R = e^{2i(\sigma_\ell + \delta^R)}$. Then the function $\Psi^R(k, r)$ is expressed as

$$\Psi^R(k, r) = \frac{1}{2i} [-\hat{U}_-^R(k, r) + S^R \hat{U}_+^R(k, r)] \quad (11)$$

in terms of Jost solutions \hat{U}_\pm^R . The latter are the solutions to the Volterra integral equations [13]

$$\hat{U}_\pm^R(k, r) = u_\ell^\pm(\eta, kr) - \int_r^\infty dr' G_\ell^C(r, r', k) V_s(r') \hat{U}_\pm^R(k, r'). \quad (12)$$

The kernel $G_\ell^C(r, r', k)$ here is given by

$$\begin{aligned} G_\ell^C(r, r', k) = \\ \frac{i}{2k} [u_\ell^+(\eta, kr) u_\ell^-(\eta, kr') - u_\ell^+(\eta, kr') u_\ell^-(\eta, kr)]. \end{aligned} \quad (13)$$

The requirement for the wave function and its derivative to obey the continuity conditions $\partial^m \Psi^R(k, R - 0) =$

$\partial^m \Psi^R(k, R + 0)$ ($m = 0, 1$) at the point $r = R$ completes the construction of Ψ^R . This construction provides a way to calculate a^R and S^R

$$\begin{aligned} -2ia^R &= W_R(\hat{U}_-^R, \hat{U}_+^R)/W_R(\hat{j}_\ell, \hat{U}_+^R), \\ S^R &= W_R(\hat{U}_-^R, \hat{j}_\ell)/W_R(\hat{U}_+^R, \hat{j}_\ell). \end{aligned} \quad (14)$$

Here $W_R(f, g)$ denotes the Wronskian $f(r)g'(r) - g(r)f'(r)$ calculated at $r = R$. The expressions for a^R and S^R become simpler when the radius R is chosen large enough. If the asymptotics $\hat{U}_\pm^R(k, R) \sim u_\ell^\pm(\eta, kR)$ can be used and at the same time $kR \gg \ell(\ell+1) + \eta^2$, then

$$a^R \sim e^{i\eta \log 2kR}, \quad S^R \sim e^{2i\eta \log 2kR}. \quad (15)$$

From this representation of S^R we get the phase shift asymptotics $\delta^R \sim \eta \log 2kR - \sigma_\ell$.

Once the wave function Ψ^R has been constructed, Eq. (5) is well defined. By imposing the boundary conditions

$$\begin{aligned} \Psi_R(k, 0) &= 0, \\ \Psi_R(k, r) &\sim \mathcal{A}_R u_\ell^+(\eta, kr), \quad r \rightarrow \infty \end{aligned} \quad (16)$$

this equation determines the remainder of the scattering wave function $\Psi_R = \Psi_\ell - \Psi^R$. The amplitude \mathcal{A}_R is given by $\mathcal{A}_R = \mathcal{A} - \mathcal{A}^R$. The representation of the amplitude \mathcal{A}_R in terms of the residual phase shift $\delta_R = \delta_\ell - \delta^R$ has the standard form

$$\mathcal{A}_R = e^{2i(\sigma_\ell + \delta^R)} \frac{e^{2i\delta_R} - 1}{2i}. \quad (17)$$

The structure of the formula (9) suggests a further simplification. If a new function Φ_R is introduced by $\Phi_R = (a^R)^{-1} \Psi_R$, then Eq. (5) transforms into

$$(H_\ell + V(r) - k^2)\Phi_R(k, r) = -V_R(r)\hat{j}_\ell(kr) \quad (18)$$

and the boundary conditions read

$$\begin{aligned} \Phi_R(k, 0) &= 0, \\ \Phi_R(k, r) &\sim (a^R)^{-1} \mathcal{A}_R u_\ell^+(\eta, kr). \end{aligned} \quad (19)$$

When $kr \gg \ell(\ell+1) + \eta^2$ the outgoing Coulomb wave u_ℓ^+ has the asymptotics [12]

$$u_\ell^+(\eta, kr) \sim e^{i(kr - \ell\pi/2 - \eta \log 2kr)}, \quad (20)$$

and the asymptotics of $\Phi_R(k, r)$ becomes simpler

$$\Phi_R(k, r) \sim (a^R)^{-1} \mathcal{A}_R e^{i(kr - \ell\pi/2 - \eta \log 2kr)}. \quad (21)$$

Furthermore, if $kR \gg \ell(\ell+1) + \eta^2$ and the asymptotics (15) applies, then the wave function asymptotics reduces to

$$\Phi_R(k, r) \sim e^{-i\eta \log 2kR} \mathcal{A}_R e^{i(kr - \ell\pi/2 - \eta \log 2kr)}. \quad (22)$$

The leading term of the amplitude \mathcal{A}_R can be calculated from the value of the wave function $\Phi_R(k, R)$ as

$$\mathcal{A}_R \sim e^{2i\eta \log 2kR} \Phi_R(k, R) e^{-i(kR - \ell\pi/2)}. \quad (23)$$

This formula gives the local representation for the amplitude.

The set of Eqs. (18,19,22) is our final formulation of the Coulomb scattering problem based on the driven Schrödinger equation with purely outgoing boundary conditions.

Green's function formalism and integral representation for \mathcal{A}_R . – The differential equation (18) with boundary conditions (19) can easily be transformed into the integral Lippmann-Schwinger equation

$$\Phi_R = -\hat{G}^R V_R \hat{j}_\ell - \hat{G}^R V_R \Phi_R. \quad (24)$$

The kernel of the integral operator \hat{G}^R is the Green's function

$$G^R(r, r', k) = \langle r | (H_\ell + V^R - k^2 - i0)^{-1} | r' \rangle.$$

It is defined by the standard expression

$$G^R(r, r', k) = \frac{1}{k} \Psi^R(k, r_<) U_+^R(k, r_>). \quad (25)$$

where $r_>(r_<) = \max(\min)\{r, r'\}$, and Ψ^R is the wave function constructed in the preceding section. U_+^R is the irregular solution to Eq. (6) with the asymptotics as $r \rightarrow \infty$

$$U_+^R(k, r) \sim u_\ell^+(\eta, kr). \quad (26)$$

This solution can be constructed by the matching procedure of the previous section. On the interval $[0, R]$ the function $U_+^R(k, r)$ has the form of the superposition of Riccati-Hankel [12] functions,

$$U_+^R(k, r) = c^R \hat{h}_\ell^-(kr) + d^R \hat{h}_\ell^+(kr). \quad (27)$$

On the interval $[R, \infty)$ one sets $U_+^R(k, r) = \hat{U}_+^R(k, r)$ (defined in Eq.(12)). The continuity conditions of the function $U_+^R(k, r)$ and its derivative over r at the point $r = R$ yield for the coefficients c^R and d^R

$$\begin{aligned} d^R &= W_R(\hat{U}_+^R, \hat{h}_\ell^-)/W_R(\hat{h}_\ell^+, \hat{h}_\ell^-), \\ c^R &= W_R(\hat{U}_+^R, \hat{h}_\ell^+)/W_R(\hat{h}_\ell^-, \hat{h}_\ell^+). \end{aligned} \quad (28)$$

If the asymptotics (26) can be applied in Eqs. (28), and if $kR \gg \ell(\ell+1) + \eta^2$, then the asymptotics for the coefficients c^R and d^R are

$$c^R \sim 0, \quad d^R \sim e^{-i\eta \log 2kR}. \quad (29)$$

Referring again to Eq. (24), the potential V_R has finite range R , hence for $r > R$ the integrals in Eq. (24) are taken on the finite interval $[0, R]$, and in Eq. (25) $r_> = r$ and $r_< = r'$. Therefore, Eq. (24) for $r > R$ is written as

$$\begin{aligned} \Phi_R(k, r) &= -\frac{1}{k} a^R U_+^R(k, r) \\ &\times \int_0^R dr' \hat{j}_\ell(kr') V(r') [\hat{j}_\ell(kr') + \Phi_R(k, r')], \end{aligned} \quad (30)$$

where relation (9) has been used. The asymptotics (26) applied to Eq. (30) leads to the desired integral representation for the scattering amplitude

$$\mathcal{A}_R = -\frac{(a^R)^2}{k} \int_0^R dr' \hat{j}_\ell(kr') V(r') [\hat{j}_\ell(kr') + \Phi_R(k, r')]. \quad (31)$$

Application of exterior complex scaling to the driven Schrödinger equation. – The success in solving the driven Schrödinger equation by the complex scaling method depends on whether the driving term vanishes for complex values of the coordinates. The driven Schrödinger equation formulation (18,19) perfectly meets this requirement since the potential in the right hand side is of finite range. Another useful observation made from representation (31) is that the scattering amplitude \mathcal{A}_R is completely determined by that part of solution Φ_R , which is restricted on the finite domain $0 \leq r \leq R$. These features make the application of the ECS method to the driven Schrödinger equation (18,19) ideally suited. Note that the ESC does not change the coordinates and the solution in the interior domain transforming only the exterior part of the wave function.

Let the ESC transformation operator

$$[W(Q, \alpha)\Psi](r) = \Psi(k, g_{Q,\alpha}(r)), \quad Q \geq R \quad (32)$$

be chosen in such a way that the transform $g_{Q,\alpha}(r)$ maps the interval $[0, Q]$ into itself and the interval $[Q, \infty)$ into a path in the upper half of the complex coordinate plane with the asymptotes $g_{Q,\alpha}(r) \sim e^{i\alpha}r$, $0 < \alpha < \pi/2$. Then it follows from Eq. (21) that the W-transformed solution to Eq. (18) $\Phi_R^W(k, r) = W(Q, \alpha)\Phi_R(k, r)$ has the asymptotics

$$\Phi_R^W(k, r) \sim (a^R)^{-1} \mathcal{A}_R e^{i[kg_{Q,\alpha}(r) - \ell\pi/2 - \eta \log 2k g_{Q,\alpha}(r)]}. \quad (33)$$

This clearly shows that

$$\lim_{r \rightarrow \infty} \Phi_R^W(k, r) = 0. \quad (34)$$

Let H_ℓ^W and V^W denote the transformed operators $W(Q, \alpha)H_\ell W^{-1}(Q, \alpha)$ and $W(Q, \alpha)VW^{-1}(Q, \alpha)$ respectively. Then W-transformed driven Schrödinger equation (18) takes the form

$$(H_\ell^W + V^W(r) - k^2)\Phi_R^W(k, r) = -V_R(r)\hat{j}_\ell(kr). \quad (35)$$

Furthermore, the W-transformed boundary conditions read

$$\Phi_R^W(k, 0) = 0, \quad \Phi_R^W(k, r) \rightarrow 0, \quad r \rightarrow \infty. \quad (36)$$

The function $\Phi_R^W(k, r)$ coincides with $\Phi_R(k, r)$ for $r \leq Q$. Therefore, if the equation (35) with zero boundary conditions (36) has been solved, then the scattering amplitude \mathcal{A}_R can be recovered by the integral representation

$$\mathcal{A}_R = -\frac{(a^R)^2}{k} \int_0^R dr' \hat{j}_\ell(kr') V(r') [\hat{j}_\ell(kr') + \Phi_R^W(k, r')], \quad (37)$$

or by the local representation

$$\mathcal{A}_R = e^{2i\eta \log 2kR} \Phi_R^W(k, R) e^{-i(kR - \ell\pi/2)}. \quad (38)$$

The subsequent phase shift δ_R is calculated from the representation (17) and reconstructs the phase shift δ_ℓ with the formula

$$\delta_\ell = \delta^R + \delta_R. \quad (39)$$

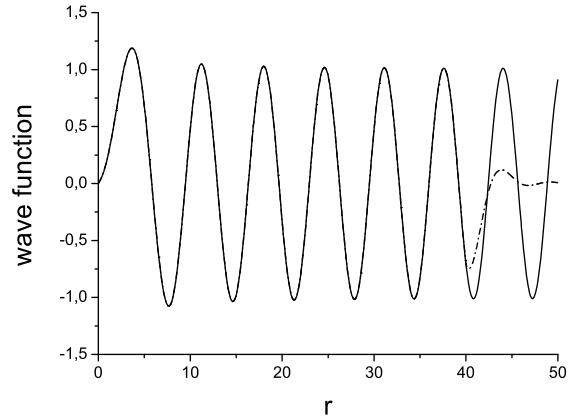


Fig. 1: The Coulomb function $F_0(1/k, kr)$ (the solid line) and the real part of the function $(\Phi_R^W(k, r) + j_0(kr))e^{i\delta R}$ (the dashed-dotted line). The momentum $k = 1$, the orbital momentum $\ell = 0$, the radius $R = 40$.

Numerical examples. – We have tested the results of the previous sections on some simple examples. As a numerical method for the solution of Eqs. (35,36), we have chosen the FEM-DVR approach described in [14]. The parameters of the numerical approximation were chosen in such a way that the numerical inaccuracies were negligible. For all the calculations presented, this was already achieved with the equally spaced finite elements of the length 1 and the Lobatto shape functions [14] of the 10th degree.

In order to introduce the boundary conditions (36) into the numerical scheme, we chose the maximal radius $R_{max} > R$, where the second condition (36) is implemented. The results get quite stable with respect to the maximal radius as soon as R_{max} is considerably larger than R . Numerical tests showed that our choice $R_{max} = 1.25R$ does not produce any noticeably errors in the results.

While the radius R and the exterior complex rotation radius Q are allowed to be different in our scheme, we have not yet found any advantages keeping them distinct. Hence, in our calculations we choose $Q = R$. The calculations have also showed that the specific choice of the ECS in Eq. (32) does not affect the results. Therefore, we have here used the sharp ECS [9]

$$g_{R,\alpha}(r) = \begin{cases} r & \text{for } r \leq R \\ R + (r - R)e^{i\alpha} & \text{for } r > R \end{cases}. \quad (40)$$

The rotation angle α was chosen to be 30 degrees.

Summarizing the description of our computational approach, we can say that the only parameter affecting the results is the radius R . All other theoretical and numerical parameters were chosen such that they do not influence the results. We first solve Eqs. (35,36) and compute the function $\Phi_R^W(k, r)$. Then we find the amplitude \mathcal{A}_R with

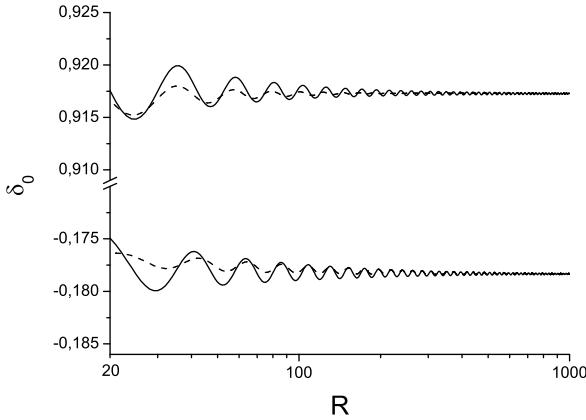


Fig. 2: The phase shift δ_0 as the function of the radius R . The integral representation (37) (the solid line) and the local representation (38) (the dashed line) are shown. The upper lines correspond to the total potential (41), the lower lines correspond to the pure Coulomb potential. The momentum $k = 3$.

the local representation (38) or with the integral representation (37). Using Eq. (17) with $\delta^R = \eta \log 2kR - \sigma_\ell$, we calculate the phase shift δ_R and finally reconstruct δ_ℓ with the relation (39).

We first compare our numerical results to the known analytic solution for the pure Coulomb potential, $V(r) = 2/r$. In Fig. 1, we display the Coulomb function $F_0(1/k, kr)$ together with the real part of the numerical solution $(\Phi_R^W(k, r) + \hat{j}_0(kr))e^{i\delta^R}$ for the radius $R = 40$ and the momentum $k = 1$. One can see that in the internal region $[0, R]$ the numerical solution practically coincides with the exact one. Hence, it can be used to determine the amplitude. Outside the internal region, for the complex rotated coordinate, the function $\Phi_R^W(k, r)$ quickly approaches zero in accordance with the second boundary condition in (36). A detailed investigation shows that the difference between the exact and numerical solutions in the internal region is evenly distributed over the whole interval $[0, R]$ and decreases when R increases.

In Figs. 2 and 3 we present the behavior of the local (38) and the integral (37) representations of the amplitude with respect to the radius R . We show results for both the pure Coulomb potential and the potential with the short range term

$$V(r) = 2/r + 15r^2e^{-r}. \quad (41)$$

In Fig. 2 one can see that the accuracies for both Coulomb potential $V(r) = 2/r$ and potential given by Eq. (41) are approximately the same. For the chosen momentum, $k = 3$, it is already as small as 1% for the relatively small radius $R = 20$. The accuracy naturally depends on both the radius R and the momentum k as we use the asymptotic expansion for $kR \rightarrow \infty$. Thus, the bigger kR is the higher is the accuracy. The phase shift approaches the exact

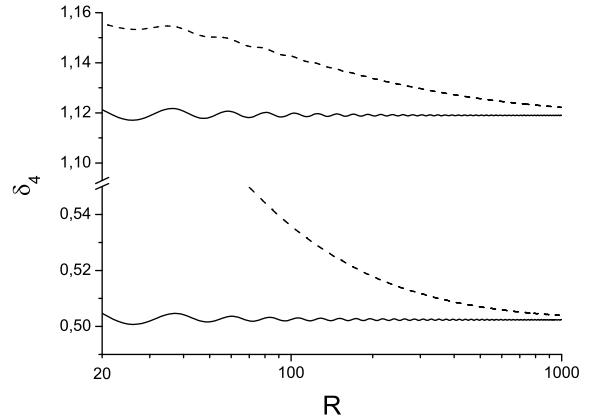


Fig. 3: The phase shift δ_4 as the function of the radius R . The notations are the same as in Fig. 2.

value when R increases while the convergence is not very fast. For zero angular momentum $\ell = 0$, the local and the integral representations give a comparable accuracy.

On comparing the data plotted in Figs. 2 and 3, there is an important difference between results for zero angular momentum and a nonzero angular momentum (here $\ell = 4$). While the accuracy given by the integral representation is about the same, the accuracy of the local representation gets worse. This lack of accuracy is due to the condition $kR \gg \ell(\ell+1) + \eta^2$ which has to be satisfied in order to use equation (22). This means that we should consider larger values of R to get the accurate result. Another possibility could be to use the next order of the asymptotic expansion with respect to kR in Eq. (19).

Finally, we have computed the s-wave scattering cross section for the potential in (41) using the present code and a highly optimized logarithmic derivative code based on the algorithm of Johnson [15]. The estimated relative accuracy of the logarithmic derivative results is smaller than 0.001. The two cross sections agree within the same limits.

Conclusions. — In this note we have presented a mathematically sound formulation which describes how the exterior complex scaling can be applied to the system with the long-range (Coulomb) interaction to compute scattering quantities. This formulation does not require any knowledge of the exact Coulomb solutions and can, therefore, be generalized to the three-body scattering problem with the charged particles. In the absence of the Coulomb potential, $\eta = 0$, our formulation also presents the rigorous justification for the ECS method [7]. This is achieved by reducing the solution of the scattering problem with a long-range (including Coulomb) potential to the solution of a boundary value problem (18,19). This reduction is exact for an arbitrary value of the radius R , and is also supplied with the exact integral representa-

tion (31) for the scattering amplitude. For large values of R , the asymptotics can be used in order to explicitly calculate the boundary conditions (19). Furthermore, the boundary problem is combined with the ECS technique as the potential in the right hand side of Eq. (18) is the finite-range potential. The numerical implementation of the theory shows both good accuracy and high efficiency of the approach.

* * *

M.V.V. and E.Y. are very thankful to Swedish Institute for support. The work of M.V.V. and N.E. is supported by a grant from the Swedish Research Council. The work of E.Y. and S.L.Y. was partially supported by the Russian Foundation for Basic Research grant 08-02-01115. S.L.Y. is thankful to Stockholm University for the support of his visit made possible under the bilateral agreement on cooperation between Stockholm University and St.Petersburg University.

REFERENCES

- [1] FADDEEV L. D. and MERKURIEV S. P., *Quantum Scattering Problem for System of Several Particles* (Kluwer, Dordrecht) 1993.
- [2] MERKURIEV S. P., *Ann. Phys.*, **130** (1980) 395.
- [3] NUTTALL J. and COHEN H. L., *Phys. Rev.*, **188** (1969) 1542.
- [4] BALSLEV E. and COMBES J. M., *Comm. Math. Phys.*, **22** (1971) 280.
- [5] MCCURDY C. W. and MARTIN F., *J. Phys. B: At. Mol. Opt. Phys.*, **37** (2004) 917.
- [6] KRUPPA A. T., SUZUKI R. and KATO K., *Phys. Rev. C*, **75** (2007) 044602.
- [7] RESCIGNO T. N., BAERTSCHY M., BYRUM D. and MCCURDY C. W., *Phys. Rev. A*, **55** (1997) 4253.
- [8] BAERTSCHY M., RESCIGNO T. N., ISAACS W. A., LI X. and MCCURDY C. W., *Phys. Rev. A*, **63** (2001) 022712.
- [9] SIMON B., *Phys. Lett. A*, **71** (1979) 211.
- [10] HISLOP P. D. and SIGAL I. M., *Introduction to Spectral Theory: With Applications to Schrödinger Operators* (Springer-Verlag New York Inc.) 1996, ch. 16, 17.
- [11] MCCURDY C. W., BAERTSCHY M. and RESCIGNO T. N., *J. Phys. B: At. Mol. Opt. Phys.*, **37** (2004) R137.
- [12] *Handbook of Mathematical Functions*, edited by ABRAMOWITZ M. and STEGUN I. (Dover, New York) 1986.
- [13] NEWTON R.G., *Scattering Theory of Waves and Particles* (Springer-Verlag, New-York) 1982.
- [14] RESCIGNO T. N. and MCCURDY C. W., *Phys. Rev. A*, **62** (2000) 032706.
- [15] JOHNSON B. R., *J. Comp. Phys.*, **13** (1973) 445
-JOHNSON B. R., *Phys. Rev. A*, **32** (1985) 1241
-MANALOPOPOULOS D. E., JAMIESON M. J. and PRADHAN A. D., *J. Comp. Phys.*, **105** (1993) 169.